[[class Notes]] 2/13

Calculating EQ concentrations from K

$COCl_2(g) \rightleftharpoons CO(g) + Cl_2(g)$ $K_P = 6.8 \times 10^{-9}$

$\downarrow$ 1 atm $\downarrow$ EQ pressure?

$$K_P = \frac{(P_{CO})(P_{Cl_2})}{(P_{COCl_2})} = 6.8 \times 10^{-9}$$

	$COCl_2$	CO	Cl_2
I	1 atm	0	0
C	$-X$	$+X$	$+X$
E	$1-X$	X	X

$$K_P = \frac{(X)(X)}{(1-X)} = \frac{X^2}{1-X} = 6.8 \times 10^{-9}$$

K is small
→ assume $1-X \approx 1$

$X^2 = 6.8 \times 10^{-9}$

$X = 8.2 \times 10^{-5}$ atm

5% "rule"

If $\frac{X}{[C]_0} \times 100 < 5\%$ (or 0.05) GOOD to GO!

initial concentration → $[C]_0$

EX) $2NOCl(g) \rightleftharpoons 2NO(g) + Cl_2(g)$ $K = 1.6 \times 10^{-5}$

1 mol / 2L flask EQ

	$NOCl$	NO	Cl_2
I	0.5M	0	0
C	$-2X$	$+2X$	$+X$
E	$0.5-2X$	$2X$	X

→

$K = \frac{[Cl_2][NO]^2}{[NOCl]^2} \rightarrow \frac{(x)(2x)^2}{(0.5-2x)^2}$ * assume $x << 0.05$

$K = \frac{4x^3}{(0.05)^2} = 1.6 \times 10^{-5}$

$x = 0.01$

IS A REACTION @ EQ?

$CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$ $K_c = 1.0$

$\downarrow$ 1M $\quad \downarrow$ 1M $\quad \downarrow$ 2M $\quad \downarrow$ 2M

calculate reactant quotient (Q)

→ Q takes same form as EQ constant K, but the values used to calculate Q are the actual current conditions

$Q = \frac{[CO_2][H_2]}{[CO][H_2O]} = \frac{(2)(2)}{(1)(1)} = 4$ $K_c = 1$

→ compare Q to K

$Q > K$, too many products, expect rxn to shift left to reactants

- If $Q < K$, rxn needs to proceed to products
- If $Q = K$, rxn is at equilibrium
- If $Q > K$, rxn proceeds to reactants

sample calculation of Q

$2NO(g) \rightleftharpoons N_2(g) + O_2(g)$ $K = 2.4 \times 10^3$

1L flask contains

0.024 moles NO

2 mol N_2

2.6 moles O_2

$Q = \frac{[N_2][O_2]}{[NO]^2} = \frac{(2)(2.6)}{(0.024)^2} = 9028$

$Q > K$, rxn shifts towards reactants (left)

Le Châteliers Principle

- If a system is @ EQ and it undergoes stress, it will respond to overcome the effect of that stress

$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$ @ EQ

- Add H_2 or I_2, the EQ shifts to right to use up added reactants
- remove HI, eq shifts to the right to make more product
- add HI, EQ shifts left to use up a added HI
- remove H_2 or I_2 shifts to left to make more reactant

- changes in pressure/volume (gasses)
  → higher volume or lower pressure favors the side of equation w/ more moles

- changes in temperature
  → is the rxn endothermic or exothermic
    ↳ endothermic: write heat as a reactant (ΔH positive)
    ↳ exothermic: write heat as a product (ΔH negative)
  → EX) $Co(H_2O)_6^{2+}(aq) + 4Cl^-(aq) \rightleftharpoons CoCl_4^{2-}(aq) + 6H_2O(l)$ $\Delta H > 0$
  +heat
  endothermic

  ← ice
  Heat →

  * ice - removing heat (reactant); heat - adding reactant